Magnetic Resonance in Solids, 2012, vol.14, N2, pages 12202-12206

NMR studies and molecular dynamics simulation of cyclosporin in complex with detergent micelles

Efimov S., Klochkov V.
Kazan Federal University, 420008, Kremlevskaya 18, Kazan, Russia

Abstract

Cyclosporin A is a highly hydrophobic peptide, but its complex with sodium dodecyl sulphate micelles can be readily dissolved in water. Nuclear magnetic resonance (NMR) investigations of cyclosporin bound to detergent micelles were carried out (including NOE spectroscopy) and yielded internuclear distances for a set of atom pairs. Based on these structural data, conformation of cyclosporin was obtained by means of molecular dynamics simulation.

Keywords

Model membrane, Molecular dynamics simulation, NOE spectroscopy, Peptide conformation